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1: J Mol Biol 1993 Feb 5;229 (3):695-706

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## Solution structure of a variant of human pancreatic secretory trypsin inhibitor determined by nuclear magnetic resonance spectroscopy.

Klaus W, Schomburg D.

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The structure of a variant of human pancreatic secretory trypsin inhibitor (PSTI) has been determined by  $^1\text{H}$  nuclear magnetic resonance (n.m.r.) spectroscopy and a combination of distance geometry and molecular dynamics simulations. After complete assignment of the  $^1\text{H}$  signals, the nuclear Overhauser data imply the existence of a rather well-determined tertiary structure stabilized by a central alpha-helix and a short three-stranded beta-sheet. The tertiary structure of the amino terminus and of the loop 11-17 could not be defined by n.m.r. data, suggesting a high flexibility in these areas. As the crystal structures of two complexes of human PSTI variants and that of an uncomplexed variant are also known a comparison of the PSTI tertiary structure in solution and in the crystal is now possible.

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